2-(2,2-Dimethylpentoxy)-3-(n-pentyl) pyrazine

Inchi: InChI=1S/C16H28N2O/c1-5-7-8-9-14-15(18-12-11-17-14)19-13-16(3,4)10-6-2/h11-12H,5

InchiKey: ZQKNMPUBCNMMQI-UHFFFAOYSA-N

Formula: C16H28N2O

SMILES: CCCCCc1nccnc1OCC(C)(C)CCC

Mol. weight [g/mol]: 264.41

CAS: 116660-27-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.45		Crippen Method
logp	4.414		Crippen Method
mcvol	238.370	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660276&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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